Formaldehyde-(14)C

3046-49-9 | DTXSID20184538

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 12.9 days

Global applicability domain: Outside

Local applicability domain index: 2.06e-01

Confidence level: 8.71e-01

Nearest Neighbors from the Training Set

Pentane
Measured: 40.7
Predicted: 6.52

Tridecane
Measured: 305
Predicted: 13.5

Tetradecane
Measured: 1370
Predicted: 18.3

Dodecane
Measured: 201
Predicted: 10.6

Pentadecane
Measured: 1810
Predicted: 20.8